Mechanoluminescence in Elastomers: Physics and Multiscale Modeling

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Abstract: Mechanoluminescence is a phenomenon where broken chemical bonds send out visible light upon stress application. To this end, special mechanophores are added into the polymer network prior to its vulcanization. As such, bis(adamantyl) 1,2-dioxetane can be used. The breakage of the dioxetane cross-linker is irreversible and can directly be used to assess the damage evolution in rubber-like materials. The intensity of the emitted light correlates with the underlying evolution of chain scission in polymers. In this contribution, an anisotropic analytical network-averaging concept [1] is utilized to model mechanoluminescence, Mullins effect, hysteresis and induced anisotropy in mechano-chemically responsive polymeric materials [2]. To this end, the polymer network is decomposed into two induced anisotropic damage networks. One of them is responsible for the chain scission and irreversible chain debonding (resulting in the Mullins effect and mechanoluminescence), while the other one describes reversible chain debonding (causing hysteresis). The network damage and recovery alter the directional distribution of molecules in space and consequently change the mean field deformation measures (mesoscopic stretch and tube contraction). The mechanoluminescence is elucidated on the basis of microvoid growth [3]. By this means, its characteristics such as the irreversibility and the anisotropy can be captured. Model predictions demonstrate good agreement with experimental data of dioxetane cross-linked and filled elastomers.

References

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